10/ 040,319

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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 20	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 23	Sep 03	JAPIO has been reloaded and enhanced
NEWS 24	Sep 16	Experimental properties added to the REGISTRY file
NEWS 25	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 26	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 27	Oct 21	EVENTLINE has been reloaded
NEWS 28	Oct 24	BEILSTEIN adds new search fields
NEWS 29	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 30	Oct 25	MEDLINE SDI run of October 8, 2002
NEWS 31	Nov 18	DKILIT has been renamed APOLLIT
NEWS 32	Nov 25	More calculated properties added to REGISTRY
NEWS 33	Dec 02	TIBKAT will be removed from STN
NEWS 34	Dec 04	CSA files on STN
NEWS 35	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 36	Dec 17	TOXCENTER enhanced with additional content
NEWS 37	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 38	Dec 30	ISMEC no longer available
NEWS 39	Jan 21	NUTRACEUT offering one free connect hour in February 2003
NEWS 40	Jan 21	PHARMAML offering one free connect hour in February 2003
NEWS 41	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 42	Feb 13	CANCERLIT is no longer being updated
NEWS 43	Feb 24	METADEX enhancements
NEWS 44	Feb 24	PCTGEN now available on STN
NEWS 45	Feb 24	TEMA now available on STN
NEWS 46	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 47	Feb 26	PCTFULL now contains images

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 NEWS 48  Mar 04  SDI PACKAGE for monthly delivery of multifile SDI results
 NEWS 49  Mar 19  APOLLIT offering free connect time in April 2003
 NEWS 50  Mar 20  EVENTLINE will be removed from STN
 NEWS 51  Mar 24  PATDPAFULL now available on STN
 NEWS 52  Mar 24  Additional information for trade-named substances without
                  structures available in REGISTRY
 NEWS 53  Mar 24  Indexing from 1957 to 1966 added to records in CA/CAPLUS

 NEWS EXPRESS  January 6 CURRENT WINDOWS VERSION IS V6.01a,
               CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

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  * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *


FILE 'HOME' ENTERED AT 10:39:40 ON 31 MAR 2003

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 10:39:58 ON 31 MAR 2003
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STRUCTURE FILE UPDATES:   30 MAR 2003  HIGHEST RN 500991-80-0
DICTIONARY FILE UPDATES:  30 MAR 2003  HIGHEST RN 500991-80-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10040319.str
```

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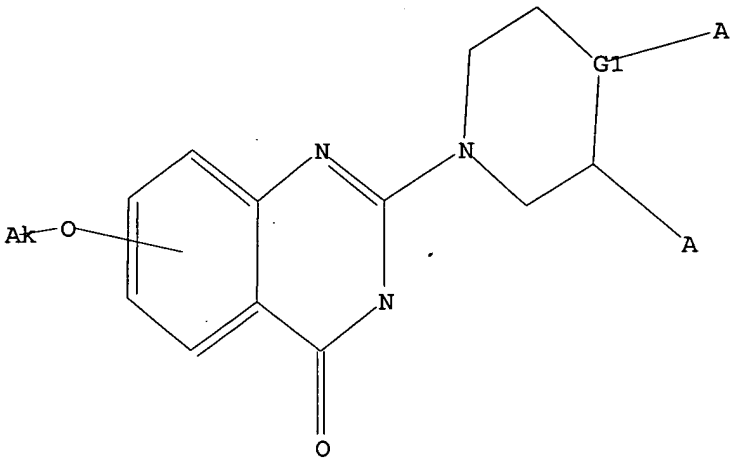
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 10:40:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 278 TO ITERATE

100.0% PROCESSED 278 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4560 TO 6560
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 10:40:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 5942 TO ITERATE

100.0% PROCESSED 5942 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

L3 9 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 148.15 148.36

FILE 'CAPLUS' ENTERED AT 10:40:38 ON 31 MAR 2003
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 31 Mar 2003 VOL 138 ISS 14
FILE LAST UPDATED: 30 Mar 2003 (20030330/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 0 L3

=> s caold
L5 3 CAOLD

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.56	150.92

FILE 'CAOLD' ENTERED AT 10:41:37 ON 31 MAR 2003
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s l3
L6 0 L3

=> d his

(FILE 'HOME' ENTERED AT 10:39:40 ON 31 MAR 2003)

FILE 'REGISTRY' ENTERED AT 10:39:58 ON 31 MAR 2003
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 9 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:40:38 ON 31 MAR 2003
L4 0 S L3
L5 3 S CAOLD

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FILE 'CAOLD' ENTERED AT 10:41:37 ON 31 MAR 2003
L6 0 S L3

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.40 151.32

FILE 'REGISTRY' ENTERED AT 10:42:11 ON 31 MAR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 MAR 2003 HIGHEST RN 500991-80-0
DICTIONARY FILE UPDATES: 30 MAR 2003 HIGHEST RN 500991-80-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d l3 1- ibib abs hitstr
'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information

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BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS --ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

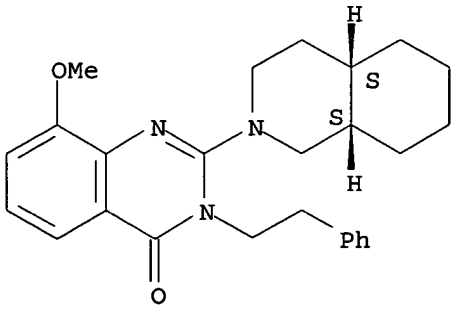
The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):reg sam fide
YOU HAVE REQUESTED DATA FROM 9 ANSWERS - CONTINUE? Y/(N):y
1 RN 319912-81-7 REGISTRY

L3 ANSWER 1 OF 9 REGISTRY COPYRIGHT 2003 ACS
IN 4(3H)-Quinazolinone, 8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-3-(2-phenylethyl)-, rel- (9CI)
MF C26 H31 N3 O2

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 319912-81-7 REGISTRY
CN 4(3H)-Quinazolinone, 8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-3-(2-phenylethyl)-, rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H31 N3 O2

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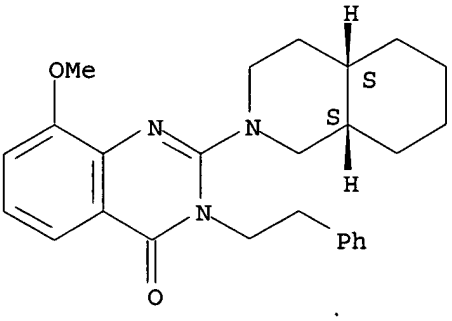
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	458	pH 1	(1) ACD
Bioconc. Factor (BCF)	2123	pH 4	(1) ACD
Bioconc. Factor (BCF)	2128	pH 7	(1) ACD
Bioconc. Factor (BCF)	2128	pH 8	(1) ACD
Bioconc. Factor (BCF)	2128	pH 10	(1) ACD
Boiling Point (BP)	577.7+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	86.48+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	303.2+/-54.2 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1805	pH 1	(1) ACD
Koc (KOC)	8364	pH 4	(1) ACD
Koc (KOC)	8385	pH 7	(1) ACD
Koc (KOC)	8385	pH 8	(1) ACD
Koc (KOC)	8385	pH 10	(1) ACD
logD (LOGD)	4.01	pH 1	(1) ACD
logD (LOGD)	4.68	pH 4	(1) ACD
logD (LOGD)	4.68	pH 7	(1) ACD
logD (LOGD)	4.68	pH 8	(1) ACD
logD (LOGD)	4.68	pH 10	(1) ACD
logP (LOGP)	4.682+/-0.941		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD

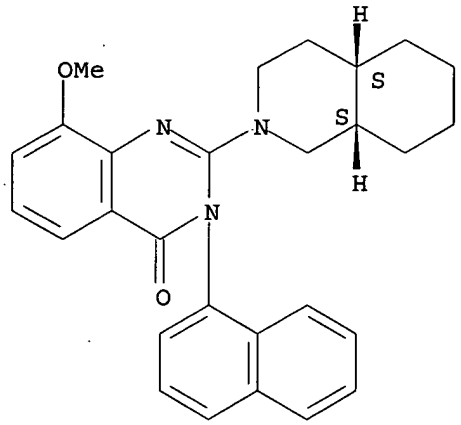
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	417.54		(1) ACD
pKa (PKA)	1.26+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	2.40E-13 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

2 RN 319912-77-1 REGISTRY

L3 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2003 ACS
IN 4(3H)-Quinazolinone, 8-methoxy-3-(1-naphthalenyl)-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI)
MF C28 H29 N3 O2

Relative stereochemistry.



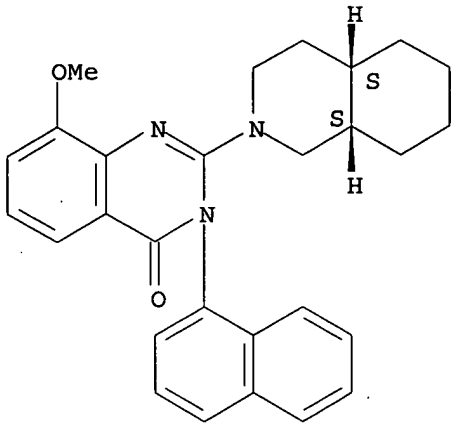
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 319912-77-1 REGISTRY
CN 4(3H)-Quinazolinone, 8-methoxy-3-(1-naphthalenyl)-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C28 H29 N3 O2
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	6810	pH 1	(1) ACD
Bioconc. Factor (BCF)	8484	pH 4	(1) ACD
Bioconc. Factor (BCF)	8486	pH 7	(1) ACD
Bioconc. Factor (BCF)	8486	pH 8	(1) ACD
Bioconc. Factor (BCF)	8486	pH 10	(1) ACD
Boiling Point (BP)	617.6+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	91.58+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	327.3+/-56.7 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	18110	pH 1	(1) ACD
Koc (KOC)	22562	pH 4	(1) ACD
Koc (KOC)	22568	pH 7	(1) ACD
Koc (KOC)	22568	pH 8	(1) ACD
Koc (KOC)	22568	pH 10	(1) ACD
logD (LOGD)	5.38	pH 1	(1) ACD
logD (LOGD)	5.47	pH 4	(1) ACD
logD (LOGD)	5.47	pH 7	(1) ACD
logD (LOGD)	5.47	pH 8	(1) ACD
logD (LOGD)	5.47	pH 10	(1) ACD
logP (LOGP)	5.473+/-0.940		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	439.55		(1) ACD
pKa (PKA)	0.36+/-0.70	Most Basic	(1) ACD
Vapor Pressure (VP)	3.49E-15 Torr	25.0 deg C	(1) ACD

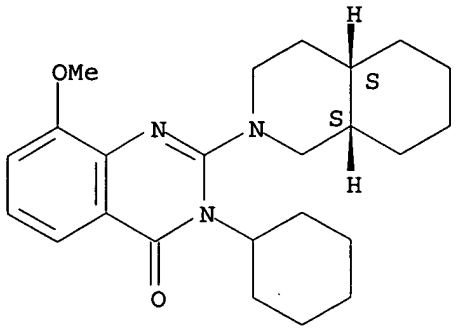
(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

3 RN 319912-71-5 REGISTRY

L3 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2003 ACS
IN 4(3H)-Quinazolinone, 3-cyclohexyl-8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-

isoquinolinyl]-, rel- (9CI)
MF C24 H33 N3 O2

Relative stereochemistry.



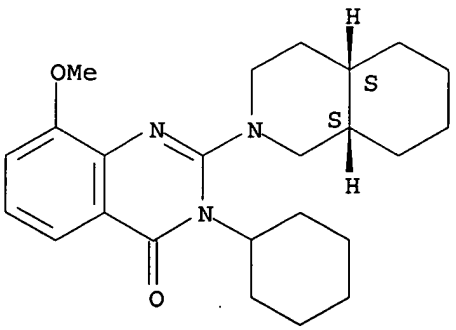
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 319912-71-5 REGISTRY
CN 4(3H)-Quinazolinone, 3-cyclohexyl-8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H33 N3 O2
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.1	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.



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Calculated Properties (CALC)

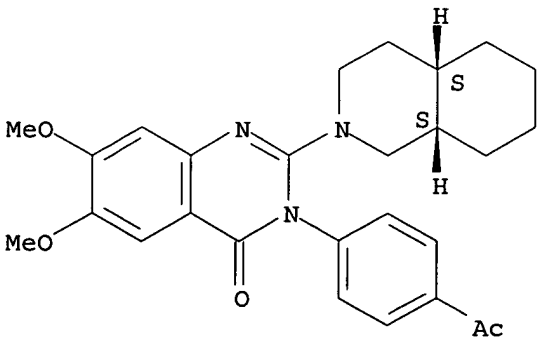
PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	318	pH 1	(1) ACD
Bioconc. Factor (BCF)	1682	pH 4	(1) ACD
Bioconc. Factor (BCF)	1687	pH 7	(1) ACD
Bioconc. Factor (BCF)	1687	pH 8	(1) ACD
Bioconc. Factor (BCF)	1687	pH 10	(1) ACD
Boiling Point (BP)	542.7+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	82.09+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	282.0+/-54.2 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1336	pH 1	(1) ACD
Koc (KOC)	7081	pH 4	(1) ACD
Koc (KOC)	7100	pH 7	(1) ACD
Koc (KOC)	7100	pH 8	(1) ACD
Koc (KOC)	7100	pH 10	(1) ACD
logD (LOGD)	3.82	pH 1	(1) ACD
logD (LOGD)	4.55	pH 4	(1) ACD
logD (LOGD)	4.55	pH 7	(1) ACD
logD (LOGD)	4.55	pH 8	(1) ACD
logD (LOGD)	4.55	pH 10	(1) ACD
logP (LOGP)	4.550+/-0.940		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	395.54		(1) ACD
pKa (PKA)	1.30+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	7.71E-12 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

4 RN 318957-21-0 REGISTRY

L3 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2003 ACS
IN 4(3H)-Quinazolinone, 3-(4-acetylphenyl)-6,7-dimethoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI)
MF C27 H31 N3 O4

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

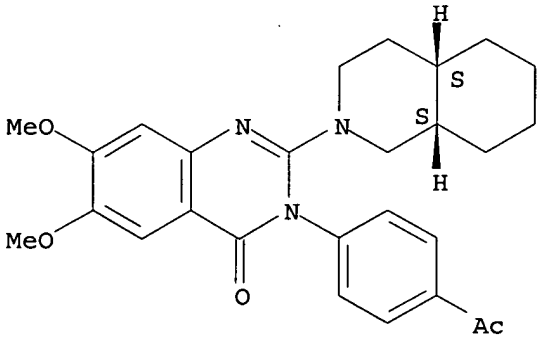
10/ 040,319

RN 318957-21-0 REGISTRY
CN 4(3H)-Quinazolinone, 3-(4-acetylphenyl)-6,7-dimethoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H31 N3 O4
SR Chemical Library

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	717	pH 1	(1) ACD
Bioconc. Factor (BCF)	727	pH 4	(1) ACD
Bioconc. Factor (BCF)	727	pH 7	(1) ACD
Bioconc. Factor (BCF)	727	pH 8	(1) ACD
Bioconc. Factor (BCF)	727	pH 10	(1) ACD
Boiling Point (BP)	632.4+/-65.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	93.50+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	336.3+/-61.7 deg C		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3833	pH 1	(1) ACD
Koc (KOC)	3887	pH 4	(1) ACD
Koc (KOC)	3887	pH 7	(1) ACD
Koc (KOC)	3887	pH 8	(1) ACD
Koc (KOC)	3887	pH 10	(1) ACD
logD (LOGD)	4.06	pH 1	(1) ACD
logD (LOGD)	4.07	pH 4	(1) ACD
logD (LOGD)	4.07	pH 7	(1) ACD
logD (LOGD)	4.07	pH 8	(1) ACD

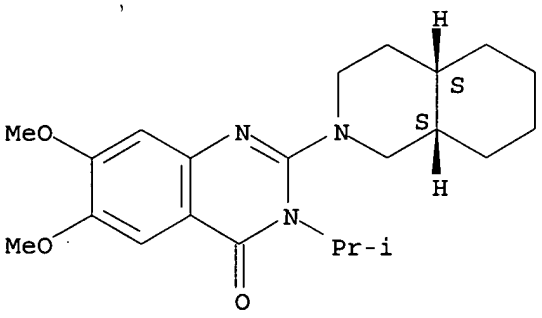
logD (LOGD)	4.07	pH 10	(1) ACD
logP (LOGP)	4.069+/-0.962		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	461.55		(1) ACD
Vapor Pressure (VP)	6.72E-16 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

5 RN 318957-19-6 REGISTRY

L3 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2003 ACS
IN 4(3H)-Quinazolinone, 6,7-dimethoxy-3-(1-methylethyl)-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI)
MF C22 H31 N3 O3

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

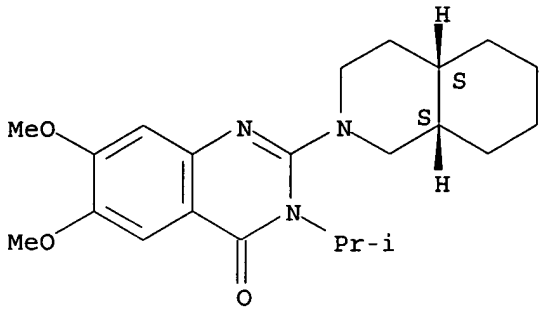
RN 318957-19-6 REGISTRY
CN 4(3H)-Quinazolinone, 6,7-dimethoxy-3-(1-methylethyl)-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H31 N3 O3
SR Chemical Library

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.

10/ 040,319



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	25.4	pH 1	(1) ACD
Bioconc. Factor (BCF)	240	pH 4	(1) ACD
Bioconc. Factor (BCF)	242	pH 7	(1) ACD
Bioconc. Factor (BCF)	242	pH 8	(1) ACD
Bioconc. Factor (BCF)	242	pH 10	(1) ACD
Boiling Point (BP)	518.3+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	79.08+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	267.3+/-56.7 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	185	pH 1	(1) ACD
Koc (KOC)	1756	pH 4	(1) ACD
Koc (KOC)	1770	pH 7	(1) ACD
Koc (KOC)	1770	pH 8	(1) ACD
Koc (KOC)	1770	pH 10	(1) ACD
logD (LOGD)	2.46	pH 1	(1) ACD
logD (LOGD)	3.44	pH 4	(1) ACD
logD (LOGD)	3.44	pH 7	(1) ACD
logD (LOGD)	3.44	pH 8	(1) ACD
logD (LOGD)	3.44	pH 10	(1) ACD
logP (LOGP)	3.440+/-0.951		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	385.50		(1) ACD
pKa (PKA)	1.91+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	7.57E-11 Torr	25.0 deg C	(1) ACD

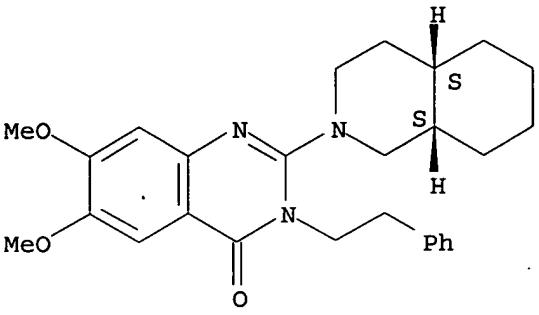
(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

6 RN 318957-16-3 REGISTRY

L3 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2003 ACS
IN 4(3H)-Quinazolinone, 6,7-dimethoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-3-(2-phenylethyl)-, rel- (9CI)
MF C27 H33 N3 O3

Relative stereochemistry.

10/ 040,319



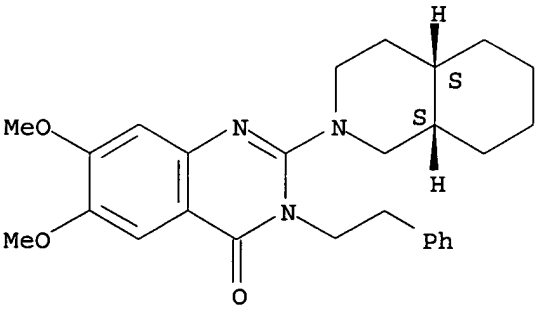
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 318957-16-3 REGISTRY
CN 4(3H)-Quinazolinone, 6,7-dimethoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-3-(2-phenylethyl)-, rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H33 N3 O3
SR Chemical Library

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	389	pH 1	(1) ACD
Bioconc. Factor (BCF)	2401	pH 4	(1) ACD
Bioconc. Factor (BCF)	2413	pH 7	(1) ACD
Bioconc. Factor (BCF)	2413	pH 8	(1) ACD
Bioconc. Factor (BCF)	2413	pH 10	(1) ACD

10/ 040,319

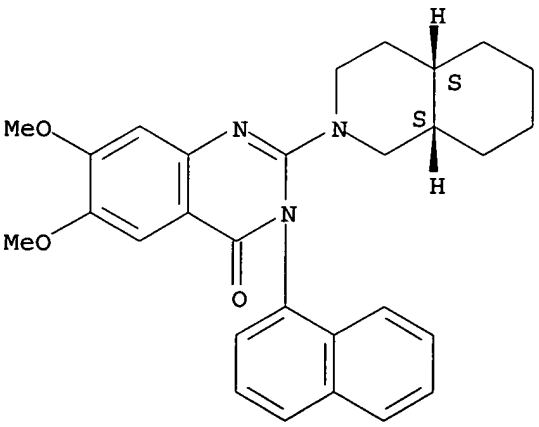
Boiling Point (BP)	604.3+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	89.86+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	319.2+/-59.2 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1480	pH 1	(1) ACD
Koc (KOC)	9127	pH 4	(1) ACD
Koc (KOC)	9173	pH 7	(1) ACD
Koc (KOC)	9173	pH 8	(1) ACD
Koc (KOC)	9173	pH 10	(1) ACD
logD (LOGD)	3.96	pH 1	(1) ACD
logD (LOGD)	4.75	pH 4	(1) ACD
logD (LOGD)	4.75	pH 7	(1) ACD
logD (LOGD)	4.75	pH 8	(1) ACD
logD (LOGD)	4.75	pH 10	(1) ACD
logP (LOGP)	4.754+/-0.951		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	447.57		(1) ACD
pKa (PKA)	1.69+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	1.49E-14 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

7 RN 318957-14-1 REGISTRY

L3 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2003 ACS
IN 4(3H)-Quinazolinone, 6,7-dimethoxy-3-(1-naphthalenyl)-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI)
MF C29 H31 N3 O3

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 318957-14-1 REGISTRY
CN 4(3H)-Quinazolinone, 6,7-dimethoxy-3-(1-naphthalenyl)-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH

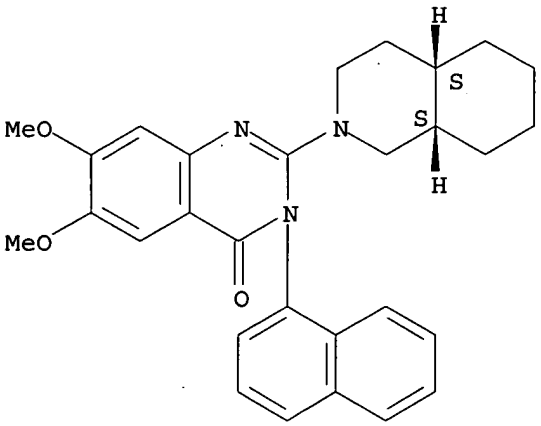
10/ 040,319

MF C29 H31 N3 O3
SR Chemical Library

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	9082	pH 1	(1) ACD
Bioconc. Factor (BCF)	9620	pH 4	(1) ACD
Bioconc. Factor (BCF)	9621	pH 7	(1) ACD
Bioconc. Factor (BCF)	9621	pH 8	(1) ACD
Bioconc. Factor (BCF)	9621	pH 10	(1) ACD
Boiling Point (BP)	640.6+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	94.58+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	341.2+/-59.2 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	23305	pH 1	(1) ACD
Koc (KOC)	24687	pH 4	(1) ACD
Koc (KOC)	24688	pH 7	(1) ACD
Koc (KOC)	24688	pH 8	(1) ACD
Koc (KOC)	24688	pH 10	(1) ACD
logD (LOGD)	5.52	pH 1	(1) ACD
logD (LOGD)	5.54	pH 4	(1) ACD
logD (LOGD)	5.54	pH 7	(1) ACD
logD (LOGD)	5.54	pH 8	(1) ACD
logD (LOGD)	5.54	pH 10	(1) ACD

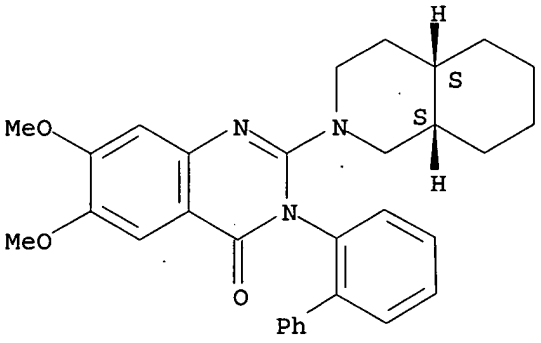
logP (LOGP)	5.545+/-0.950		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	469.57		(1) ACD
Vapor Pressure (VP)	2.62E-16 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

8 RN 318957-11-8 REGISTRY

L3 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2003 ACS
IN 4(3H)-Quinazolinone, 3-[1,1'-biphenyl]-2-yl-6,7-dimethoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI)
MF C31 H33 N3 O3

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

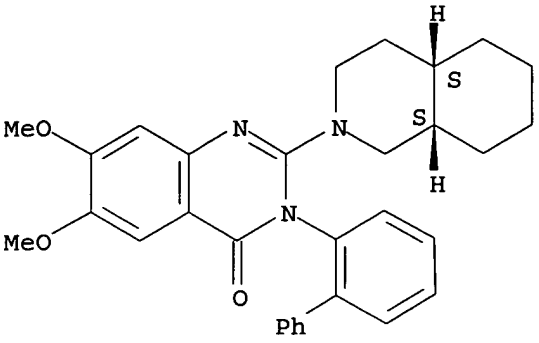
RN 318957-11-8 REGISTRY
CN 4(3H)-Quinazolinone, 3-[1,1'-biphenyl]-2-yl-6,7-dimethoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H33 N3 O3
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.

10/ 040,319



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	23295	pH 1	(1) ACD
Bioconc. Factor (BCF)	24177	pH 4	(1) ACD
Bioconc. Factor (BCF)	24178	pH 7	(1) ACD
Bioconc. Factor (BCF)	24178	pH 8	(1) ACD
Bioconc. Factor (BCF)	24178	pH 10	(1) ACD
Boiling Point (BP)	656.7+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	96.69+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	350.9+/-59.2 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	46004	pH 1	(1) ACD
Koc (KOC)	47747	pH 4	(1) ACD
Koc (KOC)	47749	pH 7	(1) ACD
Koc (KOC)	47749	pH 8	(1) ACD
Koc (KOC)	47749	pH 10	(1) ACD
logD (LOGD)	6.05	pH 1	(1) ACD
logD (LOGD)	6.07	pH 4	(1) ACD
logD (LOGD)	6.07	pH 7	(1) ACD
logD (LOGD)	6.07	pH 8	(1) ACD
logD (LOGD)	6.07	pH 10	(1) ACD
logP (LOGP)	6.071+/-0.967		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	495.61		(1) ACD
Vapor Pressure (VP)	4.04E-17 Torr	25.0 deg C	(1) ACD

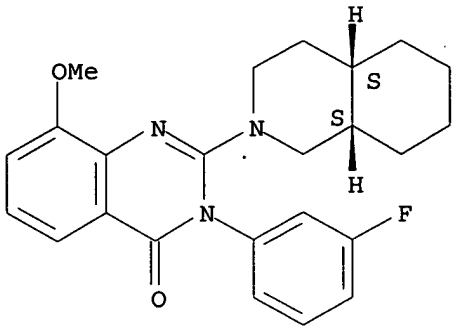
(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

9 RN 318956-79-5 REGISTRY

L3 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2003 ACS
IN 4(3H)-Quinazolinone, 3-(3-fluorophenyl)-8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI)
MF C24 H26 F N3 O2

Relative stereochemistry.

10/ 040,319



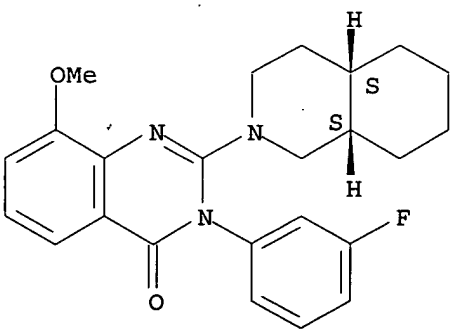
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 318956-79-5 REGISTRY
CN 4(3H)-Quinazolinone, 3-(3-fluorophenyl)-8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H26 F N3 O2
SR Chemical Library
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE

10/ 040,319

Bioconc. Factor (BCF)	1135	pH 1	(1) ACD
Bioconc. Factor (BCF)	1354	pH 4	(1) ACD
Bioconc. Factor (BCF)	1354	pH 7	(1) ACD
Bioconc. Factor (BCF)	1354	pH 8	(1) ACD
Bioconc. Factor (BCF)	1354	pH 10	(1) ACD
Boiling Point (BP)	554.3+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	83.53+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	289.0+/-56.7 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	5083	pH 1	(1) ACD
Koc (KOC)	6065	pH 4	(1) ACD
Koc (KOC)	6067	pH 7	(1) ACD
Koc (KOC)	6067	pH 8	(1) ACD
Koc (KOC)	6067	pH 10	(1) ACD
logD (LOGD)	4.35	pH 1	(1) ACD
logD (LOGD)	4.42	pH 4	(1) ACD
logD (LOGD)	4.42	pH 7	(1) ACD
logD (LOGD)	4.42	pH 8	(1) ACD
logD (LOGD)	4.42	pH 10	(1) ACD
logP (LOGP)	4.424+/-0.979		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	407.48		(1) ACD
pKa (PKA)	0.28+/-0.70	Most Basic	(1) ACD
Vapor Pressure (VP)	2.50E-12 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

=> file chemcats

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	30.70	182.02

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Fliable for any loss of profit, goodwill or any other damages arisingILE LAST UP
out of the use of this database.
For details on recent updates in CHEMCATS, enter NEWS FILE at an arrow
CHEMCATS now contains more than 5 million records. See HELP CONTENT(=>) prompt.
and NEWS FILE for details.HELP SPA, HELP SPBC, HELP SPDH, HELP SPIN, HELP SPOP,

CHEMCATS now contains more than 5 million records. See HELP CONTENT
and NEWS FILE for details.

cd liable for any loss of profit, goodwill or any other damages arising
out of the use of this database.

CHEMCATS now contains more than 5 million records. See HELP CONTENT
and NEWS FILE for details.

```
=> d his

     (FILE 'HOME' ENTERED AT 10:39:40 ON 31 MAR 2003)

     FILE 'REGISTRY' ENTERED AT 10:39:58 ON 31 MAR 2003
L1              STRUCTURE UPLOADED
L2            0 S L1
L3            9 S L1 FUL

     FILE 'CAPLUS' ENTERED AT 10:40:38 ON 31 MAR 2003
L4            0 S L3
L5            3 S CAOLD

     FILE 'CAOLD' ENTERED AT 10:41:37 ON 31 MAR 2003
L6            0 S L3

     FILE 'REGISTRY' ENTERED AT 10:42:11 ON 31 MAR 2003

     FILE 'CHEMCATS' ENTERED AT 10:46:09 ON 31 MAR 2003

=> s l3
L7            5 L3

=> d l7 1- ibib abs histstr
'IBIB' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'
'ABS' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'
'HISTSTR' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'

The following are valid formats:

The default display format is IDE.

ALL ---- AN, CO, PD, ON, CN, RN, ST, Purity, Impurity, product
         identifiers, product notes, STR, product text
         (properties, regulatory information, references, prices,
         warnings, miscellaneous fields), CO, CA, CY, TX
         (products, terms, and conditions; products and services;
         packaging and shipping; safety and handling; other
         supplier information)
COMP --- AN, CO, PD, CO, TX
IDE ---- AN, CO, PD, ON, CN, RN, LSF, ST, STR
MISC --- AN, miscellaneous product information fields
PINFO -- AN, pricing information text
PRICE -- AN, prices, quantities
PROD --- AN, product text
PROP --- AN, properties
```

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REF ---- AN, references
REGS --- AN, regulatory information
SAFE --- AN, product warnings
SINFO -- AN, safety text
HIT ---- All fields containing hit terms
KWIC --- All hit terms plus 20 words on either side
OCC ---- List of display fields containing hit terms

Hit terms will be highlighted in all displayable fields.

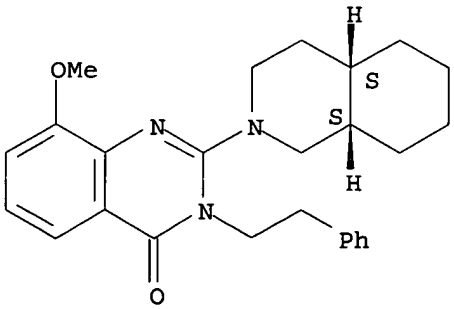
To display a particular field or fields, enter the display field codes. For a list of display field codes, enter 'HELP DFIELDS' at an arrow prompt (=>). Examples include: 'KWIC'; 'CN RN'; 'IDE CO'. You may specify the formats and fields in any order, and the information will be displayed in the same order as the format specification.

The same formats (except for HIT, KWIC, and OCC) may be used with the DISPLAY ACC command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (IDE):all
YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y

L7 ANSWER 1 OF 5 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2001:187968 CHEMCATS
Catalog Name (CO): Chem.Folio
Publication Date (PD): 15 May 2001
Order Number (ON): TRG10400#06028-D
Chemical Name (CN): 4(3H)-Quinazolinone, 8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-3-(2-phenylethyl)-, rel-
CAS Registry No. (RN): **319912-81-7**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

Relative stereochemistry.



PRICES

Quantity : milligram quantities, Price: contact supplier

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Japan

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Fax: 03-3419-9179

L7 ANSWER 2 OF 5 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2001:187964 CHEMCATS
Catalog Name (CO): Chem.Folio
Publication Date (PD): 15 May 2001
Order Number (ON): TRG10400#06027-D
Chemical Name (CN): 4(3H)-Quinazolinone, 8-methoxy-3-(1-naphthalenyl)-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel-
CAS Registry No. (RN): **319912-77-1**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

Relative stereochemistry.

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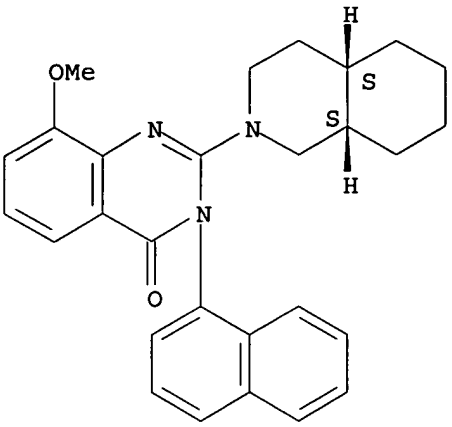

PRICES

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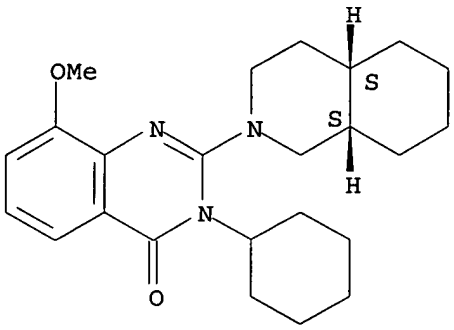
L7 ANSWER 3 OF 5 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2001:187958 CHEMCATS
Catalog Name (CO): Chem.Folio
Publication Date (PD): 15 May 2001
Order Number (ON): TRG10400#06025-D
Chemical Name (CN): 4(3H)-Quinazolinone, 3-cyclohexyl-8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel-
CAS Registry No. (RN): **319912-71-5**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

Relative stereochemistry.



PRICES

Quantity : milligram quantities, Price: contact supplier

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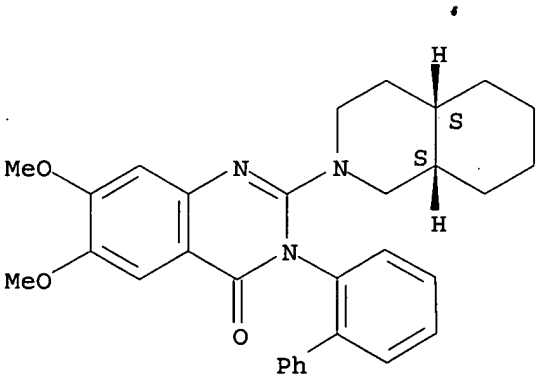
L7 ANSWER 4 OF 5 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2001:183634 CHEMCATS
Catalog Name (CO): Chem.Folio
Publication Date (PD): 15 May 2001
Order Number (ON): TRG10400#06122-D
Chemical Name (CN): 4(3H)-Quinazolinone, 3-[1,1'-biphenyl]-2-yl-6,7-dimethoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel-
CAS Registry No. (RN): **318957-11-8**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

Relative stereochemistry.



PRICES

Quantity : milligram quantities, Price: contact supplier

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L7 ANSWER 5 OF 5 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2001:183602 CHEMCATS
Catalog Name (CO): Chem.Folio
Publication Date (PD): 15 May 2001
Order Number (ON): TRG10400#06032-D
Chemical Name (CN): 4(3H)-Quinazolinone, 3-(3-fluorophenyl)-8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel-
CAS Registry No. (RN): **318956-79-5**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

Relative stereochemistry.

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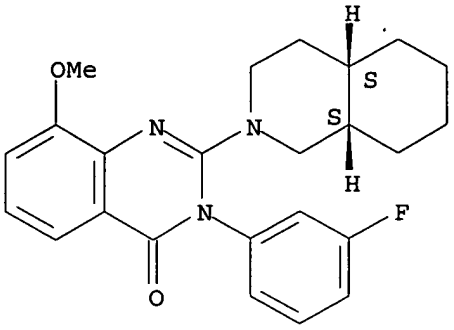

late

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Quantity : milligram quantities, Price: contact supplier

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```
=> file caplus
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                        18.64     200.66

FILE 'CAPLUS' ENTERED AT 10:47:33 ON 31 MAR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 31 Mar 2003  VOL 138 ISS 14
FILE LAST UPDATED: 30 Mar 2003  (20030330/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> d his

     (FILE 'HOME' ENTERED AT 10:39:40 ON 31 MAR 2003)

     FILE 'REGISTRY' ENTERED AT 10:39:58 ON 31 MAR 2003
L1                STRUCTURE UPLOADED
L2            0 S L1
L3            9 S L1 FUL

     FILE 'CAPLUS' ENTERED AT 10:40:38 ON 31 MAR 2003
L4            0 S L3
L5            3 S CAOLD

     FILE 'CAOLD' ENTERED AT 10:41:37 ON 31 MAR 2003
L6            0 S L3

     FILE 'REGISTRY' ENTERED AT 10:42:11 ON 31 MAR 2003

     FILE 'CHEMCATS' ENTERED AT 10:46:09 ON 31 MAR 2003
L7            5 S L3

     FILE 'CAPLUS' ENTERED AT 10:47:33 ON 31 MAR 2003

=> s l7
L8            0 L3

=> file casreact
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.83     201.49
```

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FILE 'CASREACT' ENTERED AT 10:48:53 ON 31 MAR 2003
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1907 - 30 Mar 2003 VOL 138 ISS 13

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

```
=> s l3
L9            0 L3

=> d his

     (FILE 'HOME' ENTERED AT 10:39:40 ON 31 MAR 2003)

     FILE 'REGISTRY' ENTERED AT 10:39:58 ON 31 MAR 2003
L1               STRUCTURE UPLOADED
L2             0 S L1
L3             9 S L1 FUL

     FILE 'CAPLUS' ENTERED AT 10:40:38 ON 31 MAR 2003
L4             0 S L3
L5             3 S CAOLD

     FILE 'CAOLD' ENTERED AT 10:41:37 ON 31 MAR 2003
L6             0 S L3

     FILE 'REGISTRY' ENTERED AT 10:42:11 ON 31 MAR 2003

     FILE 'CHEMCATS' ENTERED AT 10:46:09 ON 31 MAR 2003
L7             5 S L3

     FILE 'CAPLUS' ENTERED AT 10:47:33 ON 31 MAR 2003
L8             0 S L7

     FILE 'CASREACT' ENTERED AT 10:48:53 ON 31 MAR 2003
L9             0 S L3

=> log y
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                              ENTRY    SESSION
FULL ESTIMATED COST                           25.80     227.29

STN INTERNATIONAL LOGOFF AT 10:49:53 ON 31 MAR 2003
```